Bornyl acetate 375

		•		
76-49-3	3	DTXSID70	41	6

Model Performance

Model	Data

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.72	51.8	0.74	50.3	0.73	52.7	

Model Results

Predicted value: 32.0 °C

Global applicability domain: Inside

Local applicability domain index: 6.37e-01

Confidence level: 5.09e-01

Nearest Neighbors from the Training Set

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Bornyl acetate Measured: 29.0 Predicted: 32.0 Image not found

Isobornyl acrylate Measured: 97.0 Predicted: 59.3 Image not found

Cyclohexanone, 4-methyl-

Measured: -40.6 Predicted: -15.0

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Cyclohexanone Measured: -31.0 Predicted: -14.3